National Aeronautics and Space Administration

Derived Meteorological Products for Solar Occultation Satellite Datasets and Applications to Aura Validation

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1 Derived Meteorological Products: Motivation and Description

Derived Meteorological Product (DMP) files have been produced for solar occultation (SO) satellite datasets; they include potential temperature, horizontal winds, potential vorticity (PV), equivalent Latitude (EqL), vortex edge criteria, tropopause heights, and other useful quantities derived from gridded meteorological data. These are designed to:

- Facilitate validation of non-coincident measurements by allowing comparison of air experiencing similar meteorological conditions
- Assist in studies using vortex-centered coordinates
- Aid in combining multiple datasets for detailed scientific studies

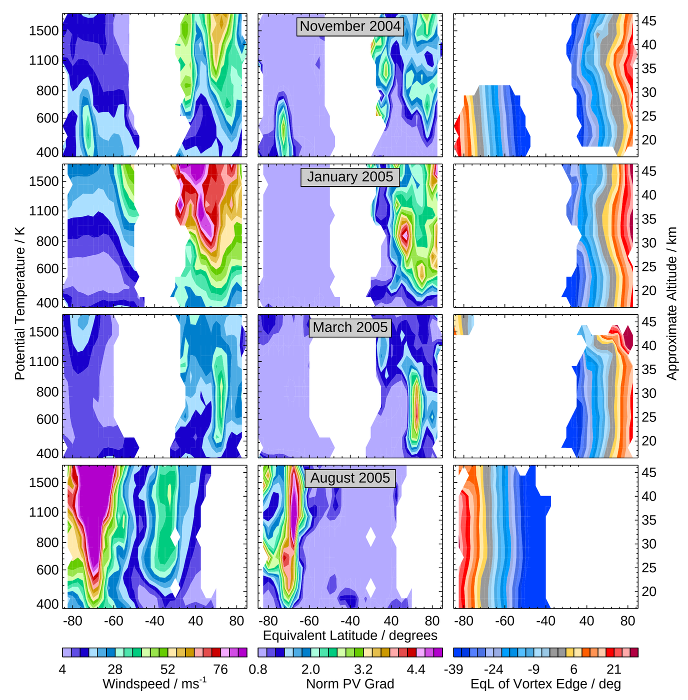
DMPs have been calculated for:

- ACE-FTS (Atmospheric Chemistry Experiment-Fourier Transform Spectrometer), from GEOS-4 (NASA Global Modeling and Assimilation Office's Goddard Earth Observing System Version 4.03) and UK Met Office (MetO) analyses
- SAGE (Stratospheric Aerosol and Gas Experiment) II & III from MetO analyses (and NCEP/CPC (National Centers for Environmental Prediction/ Climate Prediction Center) for SAGE II)
- HALOE (Halogen Occultation Experiment) from MetO analyses (preliminary, see below)
- POAM (Polar Ozone and Aerosol Measurement) II & III from MetO analyses
- Similar products derived from MetO analyses can be provided for user-defined data locations
- DMPs for SAGE II/III, HALOE, and POAM II/III are publicly available (see section 5); ACE-FTS DMPs are provided to the ACE Science Team to distribute as they choose

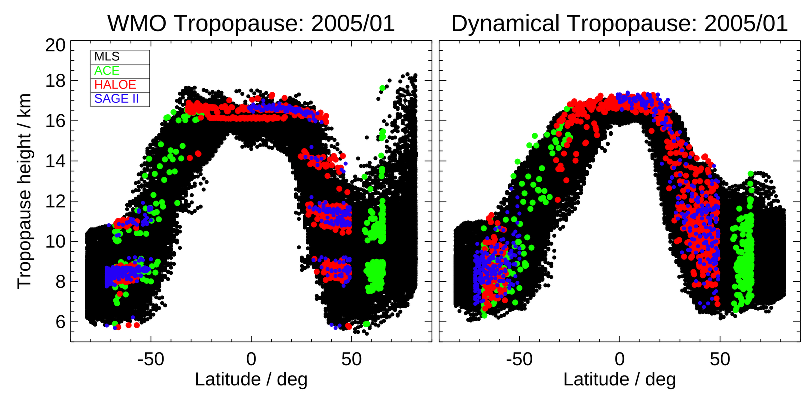
DMPs are summarized in the Table (far right):

- Quantities given in blue are directly interpolated, in purple are from the instruments' observing geometry; other quantities are calculated from information in meteorological datasets
- 2D products are a function of altitude at each observation location; 1D are single value for each observation.
- Line-of-sight (LOS) information is not currently available for ACE and HALOE, thus quantities in gray are not available for those instruments
- This geolocation information, along with pressure provided in the instruments' data files, is used to interpolate meteorological data and derived quantities to the observation locations

- Preliminary HALOE DMPs use scalar latitudes/longitudes given in HALOE data files rather than altitude-dependent information; at levels below where HALOE file provide pressure (p), it is currently estimated from the altitude (z) using $z = (7.0\mathrm{km})\ln(p_{sfc}/p)$
- Temperature, geopotential height, horizontal winds interpolated bilinearly in the horizontal and linearly in log(p) in the vertical to SO observation locations
- Horizontal and LOS temperature gradients are calculated using the temperature field at the pressure of each observation
- Other 2D quantities (related to PV) are interpolated linearly in log(θ) in the vertical, and gradients are calculated on the θ surface of the observation
- Scaled PV (sPV) is in "vorticity units" [Dunkerton and Delisi, 1986, JGR], as described by Manney, et al [1994, JAS]



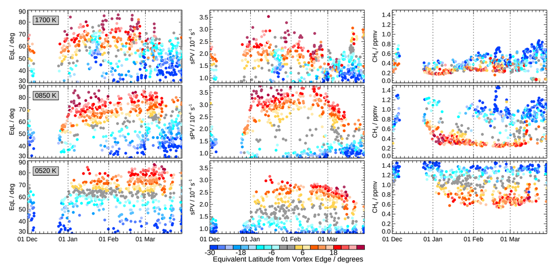
- EqL of the vortex edge center and inner and outer boundaries are calculated as the location of the maximum of (windspeed)×(normalized PV gradient):
  - The preceding figure shows vortex characteristics from ACE DMP files for Nov 2004, Jan 2005, Mar 2005, Aug 2005
  - The vortex edge has high windspeeds & strong PV gradients
  - The distance in EqL of the observation from vortex edge center is given in the DMP files
  - November shows developing NH vortex, decaying SH vortex
  - March shows early SH upper stratospheric vortex formation; top of upper tropospheric subtropical jet is misidentified as vortex
- Tropopause heights are calculated from temperature or PV profiles after interpolation to the SO locations:
  - "Dynamical" tropopause – altitude of 3.5×10^{-6} K m^2 kg^{-1} s^{-1} PV contour in the extratropics; joined to 380 K potential temperature surface in the tropics
  - Temperature gradient (WMO) tropopause – the lowest altitude at which the magnitude of the lapse rate drops below 2 K/km and remains below that value for at least 2 km – calculated as in Reichler, et al. [2003, GRL]
  - Figure below shows tropopause heights from MetO DMPs in January 2005 for MLS and several SO instruments



Derived Meteorological Product Fields		
Field	Units	Description
Alt	km	(2D) Altitudes
Lat	deg	(2D) Latitudes as a function of Altitude
Lon	deg	(2D) Longitudes as a function of Altitude
Sun Dir	deg cw from N	(2D) Line-of-Sight angle (LOS)
θ	K	(2D) Potential Temperature from met data
Temperature	K	(2D) Temperature from meteorological data
Hor T Grad	K/km	(2D) Horizontal temperature gradient
LOS T Grad	K/km	(2D) Temperature gradient along LOS
Geop Hgt	m	(2D) Geopotential Height
Zonal Wind	m/s	(2D) Zonal Wind
Merid Wind	m/s	(2D) Meridional Wind
PV	10^{-4} K m^2 kg^{-1} s^{-1}	(2D) Potential Vorticity
Scaled PV	10^{-4} s^{-1}	(2D) Scaled PV, in "vorticity units"
EqL	deg	(2D) Equivalent Latitude
Hor PV Grad	–	(2D) Normalized horizontal PV gradient
LOS PV Grad	(10^{-4} K m^2 kg^{-1} s^{-1})/km	(2D) PV gradient along LOS
EqL - VEC	deg	(2D) Distance (EqL) from vortex edge center
EqL - VEI	deg	(2D) Distance (EqL) from inner vortex edge
EqL - VEO	deg	(2D) Distance (EqL) from outer vortex edge
Dyn Tropopause	km	(1D) Dynamical tropopause altitude (3.5 PVU)
TG Tropopause	km	(1D) WMO tropopause altitude

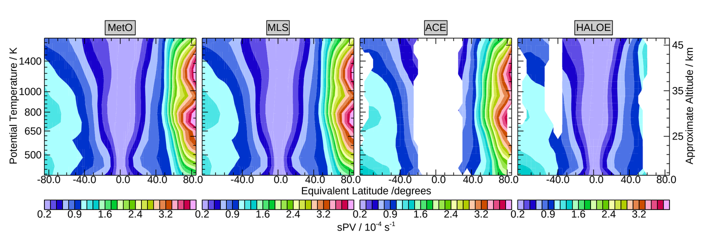
2 DMP Issues and Caveats

2.1 Vortex Edge Caveats



- Many caveats on automated vortex edge definition
- Above figure shows vortex edge as a function of EqL, sPV, CH_4
- Note clear correspondence with EqL, sPV, tracers (e.g., CH_4) in middle and lower stratosphere; vortex breakup in early to mid-March blurs these distinctions
- Several methods, including Nash [1996], produced similar results for the mid-winter middle to lower stratosphere. In the upper stratosphere, and in fall and spring, results vary, and vortex structure is often too complex for automated definitions to be useful

2.2 Sampling Issues



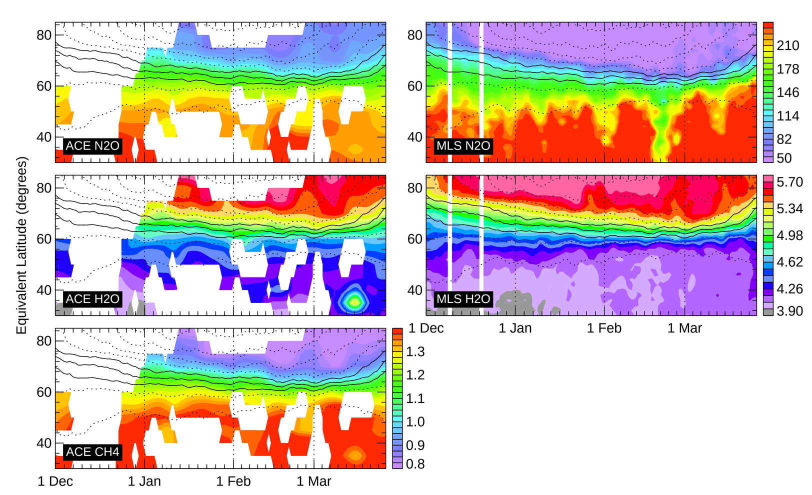
- Preceding figure shows sPV gridded in EqL/theta space as sampled by ACE, HALOE and MLS, along with values from the original MetO file
- Sampling effects can cause confusing results, especially in regions of strong tracer gradients, such as along the vortex edge
- MLS, with global daily sampling, gives values very similar to original gridded file
- HALOE, sampling only to edge of vortex region, shows weaker gradients, lower values at highest EqLs covered
- See other examples in O_3 and $ClONO_2$ plots shown in sections 3 and 4

2.3 Meteorological Datasets

- Results can differ significantly for different meteorological datasets, especially in regions of strong PV gradients, affecting quantities such as EqL and vortex edge criteria
- For long-term records, all of the meteorological datasets have changes in assimilation/analysis systems and input data; thus care must be taken in trend or variability studies that discontinuities in the meteorological data are not introduced into the analyses
- DMPs will be calculated from GEOS-4 as well as Met Office for all SO datasets, and from other analyses for some; comparisons of these will help quantify these effects

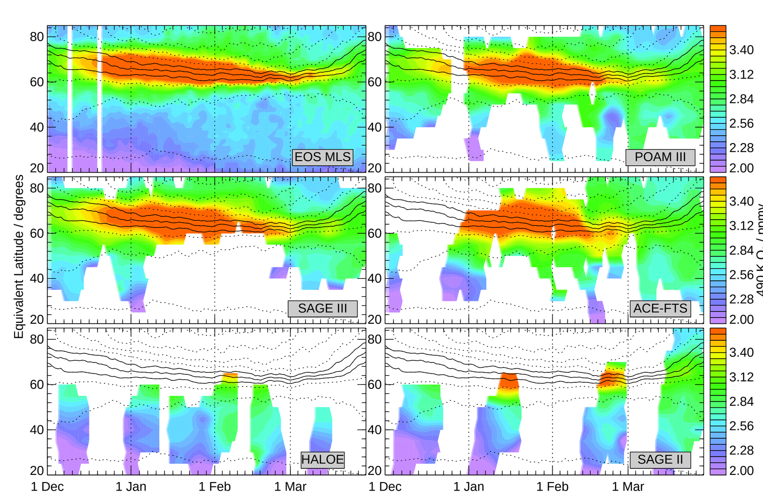
3 Examples from the 2004-2005 Arctic Winter: Comparing MLS and SOSST Data Using DMPs

DMPs such as PV and EqL are invaluable in intercomparing datasets with different sampling [e.g., Manney, et al, 2001, JGR]. The following figures show examples comparing MLS with SO observations in the 2004-2005 Arctic winter. DMPs for MLS are currently from files with a subset of the products produced for external use, but more complete versions may be made publicly available in the future.



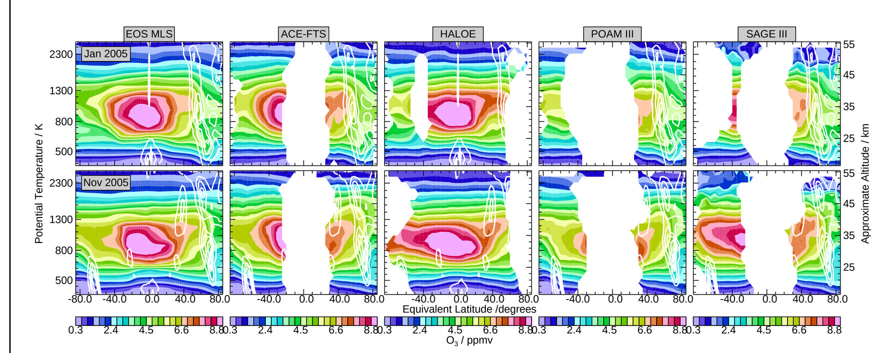
- Above figure show EqL/time plots of ACE and MLS long-lived tracer data in the lower stratosphere gridded using DMPs, N_2O (top), H_2O (center), and ACE CH_4 (bottom left)
- Gridding in EqL using DMPs shows the full extent of ACE "condition-space" coverage, maximizing information we can get from these sparse measurements

- Time evolution of ACE and MLS long-lived tracers agrees well, and ACE CH_4 evolution is consistent with that of N_2O and H_2O; some apparent biases may be sampling related (e.g., higher ACE values in vortex core)
- Both ACE and MLS show evidence of intrusions and mixing into the vortex (e.g., late February)
- Increasing (decreasing) N_2O & CH_4 (H_2O) after early February indicate descent is no longer the dominant transport process



- O_3 from MLS and SOSST instruments (above figure) shows very similar evolution and morphology

- Higher SAGE II values near vortex center in late March likely result from sampling effects related to physical location being at lower latitude
- All instruments that sample vortex show steady declines throughout the vortex from late January through early March
- Vortex ozone increases through mixing after about 10 March

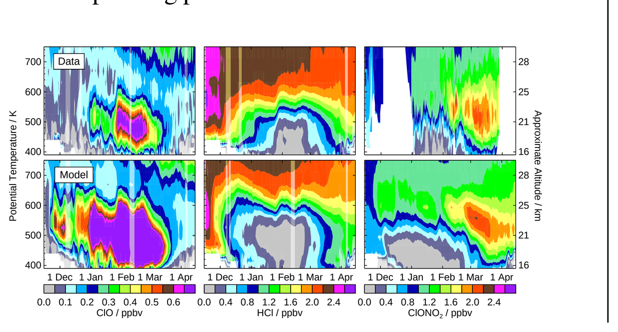


- Monthly EqL-Theta plots of O_3 from MLS and SO instruments for January and November 2005 (above figure) show broad overall agreement
- Best agreement in regions with good sampling by SO instruments (e.g., MLS and HALOE in tropics, MLS and ACE in highest EqLs)
- Sampling effects very evident for chemically active species:
  - HALOE in SH (NH) in November (January) too high near peak, since values at high EqL are coming from lower latitudes
  - POAM mid-EqL values low because coming from higher latitudes

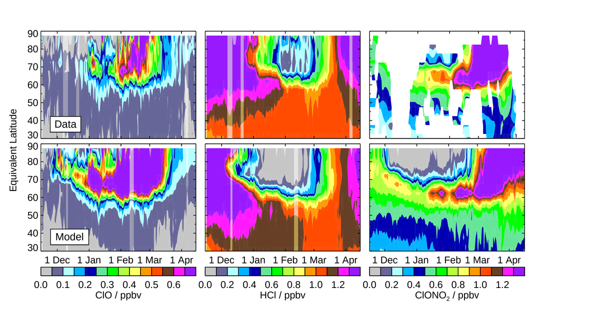
4 Combining MLS and SOSST Data For Science Studies

DMP information aids in combining measurements from instruments with very different sampling. Examples below show work from a detailed data/modeling study of chlorine partitioning [Santee et al, in preparation] combining ACE and MLS data:

- Vortex-averaged MLS ClO and HCl, and ACE $ClONO_2$, and corresponding plots from SLIMCAT CTM simulation:



- EqL/Time plots of MLS ClO and HCl, and ACE $ClONO_2$, and corresponding plots from SLIMCAT CTM simulation:



- Model and measurements show broad agreement
- ACE $ClONO_2$ shows sampling effects, e.g., high vortex average in early February is partly due to ACE sampling in "collar" along vortex edge

- Significant chlorine activation begins by mid-December
- Both model and measurements show substantial recovery into $ClONO_2$ by early February, into HCl only after early March

Other examples comparing/combining MLS and ACE data are shown in a poster on the 2006 Stratospheric Sudden Warming [Manney, et al, this session]

We invite anyone who is interested to use the publicly available DMPs, and hope that they will be useful to you. For questions/comments/problems with these products, contact

- Gloria Manney: Gloria.L.Manney@jpl.nasa.gov
- William H. Daffer: William.H.Daffer@jpl.nasa.gov

We would appreciate it very much if those who use the DMPs and find them valuable would let us know how they are using them, inform us of any publications using them, and include an acknowledgment in those publications.

5 Distribution & Data Formats

- DMPs for publicly available datasets can be obtained via anonymous ftp at JPL on mls.jpl.nasa.gov; table below summarizes locations
- Links to these DMPs will be available on new MLS website [Knosp, et al poster, session 1]
- Information on data formats and/or example read routines are provided on the ftp site for each product
- DMPs from Met Office data can also be obtained at user defined locations that are provided to us in a specified format

Availability of DMPs via FTP	
Mission/Instrument	*Location*[1]
ACE-FTS	Distributed by ACE team[2]
SAGE II	sage2/v5.0/{NCEPPV,MetOPV}
SAGE III	sage3/v03.00/dmp/g3asmb/v1.1/<y>/<d>[4]
POAM II[4]	poam2/v6.00/dmp/v1.0
POAM III[4]	poam3/v4.00/dmp/v1.0
HALOE[4]	haloe/v19/dmp/v1.0/<y>

[1]Relative to pub/outgoing/manney after logging in via FTP
[2]DMPs pushed to uwaterloo.ca and distributed from there
[3]<y>=4-digit year, <d>=3-digit day-of-year
[4]DMPs prior to August 2004 coming soon

- Most data formats mimic the format of the SO occultation dataset they are produced for
- The exception is POAM, where the mission-long files were not practical for the DMP calculations; POAM DMPs are thus in a simple IEEE binary format similar to that used for the SAGE II DMPs and dataset

6 Future Plans: DMP Improvements, Studies

6.1 Further Calculations

- Produce HALOE DMPs using full geolocation information as a function of altitude and more accurate pressure estimation at low altitude
- Calculate DMPs for all instruments (and at user-defined locations) from GEOS-4 meteorological data in addition to Met Office
- Complete historical record of POAM and HALOE DMPs

6.2 Documentation, Validation, Science Studies

- More detailed documentation based on the material in this poster will be in a paper planned for the Aura validation special issue
- This paper will also focus on more complete examples of intercomparisons with MLS data, to contribute to the work on non-coincident validation of those data

- We hope that the DMPs will be used by/useful to others for more detailed non-coincident validation studies
- Several science studies are using DMPs to combine MLS with solar occultation datasets:
  - Santee, et al., "A study of stratospheric chlorine partitioning in the winter polar vortices based on new satellite measurements and modeling", paper in preparation
  - Manney, et al., "Transport during the January/February 2006 Stratospheric Major Warming from Aura MLS and ACE-FTS data", paper in preparation, and poster, this session
  - Studies of stratopause structure and evolution, and transport across the stratopause
  - Studies of transport/chemistry during vortex development